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Valence band structure of ultrathin silicon and germanium channels in metal-oxide-semiconductor field-effect transistors

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The ultrathin body (UTB) silicon-on-insulator metal-oxide-semiconductor field-effect transistor (MOSFET) is promising for sub-50-nm complementary metal-oxide semiconductor technologies. To explore a high-mobility channel for this technology, this paper presents an examination of Si and Ge hole sub-band structure in UTB MOSFETs under different surface orientations. The dependence of the hole subband structure on the film thickness (T_{Body}) was also studied in this work. We found that the valence-band mixing in the vicinity of the zone center Γ is strongly dependent on T_{Body} for both Si and Ge, particularly for the $\langle 110 \rangle$ surface orientation. This gives rise to the following two phenomena that crucially affect the electrical characteristics of p -MOSFETs: (1) an anomalous increase of quantization mass for $\langle 110 \rangle$ Si and Ge surfaces as T_{Body} is scaled below 5 nm. (2) The dependence of energy dispersion and anisotropy on T_{Body} especially for the $\langle 110 \rangle$ surface, which advantageously increases hole velocity along the $[011]$ channel as T_{Body} is decreased. The density of states for different surface orientations are also calculated, and show that—for any given surface orientation—Ge has a smaller density of states than Si. The Ge $\langle 110 \rangle$ surface has the lowest density of states among the surface orientations considered. © 2005 American Institute of Physics. [DOI: 10.1063/1.1948528]

I. INTRODUCTION

The ultrathin body (UTB) silicon-on-insulator (SOI) metal-oxide-semiconductor field-effect transistor (MOSFET) is a promising candidate for the development of sub-50-nm complementary metal-oxide semiconductor (CMOS) technologies.¹ However, recent experimental work^{2,3} has reported serious mobility degradation in Si UTB MOSFETs with T_{Body} less than 5 nm. This may present significant limitations to achieving ballistic transport in Si UTB MOSFET devices^{4,5} with a sub-10-nm gate length.^{6,7} To counteract this problem, several notable efforts are being made to implement a higher mobility channel. Ge UTB p -MOSFET devices with a T_{Body} of 4.5 nm have been fabricated using the local condensation techniques,⁸ with large mobility improvement over Si MOSFETs. The technology for fabricating n -MOSFET and p -MOSFET devices on hybrid substrates⁹ along their optimum surfaces and channel orientations has also been demonstrated.⁹ To further this effort, it is of paramount importance to understand the band-structure characteristics of these thin-film channels, especially for the case of complicated valence bands. In the dissipative transport regime, it is advantageous to select and orient the band structure to yield a smaller two-dimensional (2D) density-of-

states mass (m_D) and conductivity mass (m_C).¹⁰ However, from a current overdrive point of view,¹¹ a larger m_D is more desirable. A large quantization mass (m_Z) is also pertinent for the suppression of surface-roughness scattering for UTB MOSFETs with a sub-5-nm T_{Body} .¹²

The purpose of this article is to provide a detailed examination of the impact of T_{Body} on the hole subband structure of Si and Ge with sub-10-nm T_{Body} and discuss its implications for carrier transport attributes in its relation to their effective m_D , m_C and m_Z . The valence-band structure is calculated via the six-band Luttinger–Kohn Hamiltonian¹³ for Si and Ge with common surface orientations— $\langle 100 \rangle$, $\langle 110 \rangle$, and $\langle 111 \rangle$ —using a triangular-well approximation¹⁴ and assuming an infinite potential barrier for the oxides at both interfaces of the semiconductors. In the following section, we will first consider the effect of coupling with the conduction band of type Γ_2^- and its implications on the use of a six-band Hamiltonian¹³ description for band-structure calculation. Section III presents a brief outline of the numerical approach employed. In Sec. IV, we will provide an assessment of the energy quantization effect for the various surface orientations and its dependency on film thickness. Section V examines the energy anisotropy of the various Si and Ge thin films. Section VI concludes with a calculation of their 2D density of states.

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TABLE I. Numerical values of bulk parameters used for the valence-band Hamiltonian for Si and Ge are obtained from Ref. 15. The Kane energy E_p , energy-gap E_G , and spin-orbit splitting Δ are given in units of eV. γ_j ($j=1,2,3$) are Luttinger parameters and m_c is the effective mass (in units of free electron mass, m_0) at the band edge of type Γ_2^- , modified Luttinger parameter (not listed in table) for eight-band Hamiltonian can be calculated from Ref. 15.

	γ_1	γ_2	γ_3	E_G	Δ	E_p	m_c
Si	4.285	0.339	1.446	4.185	0.044	21.60	0.528
Ge	13.38	4.24	5.69	0.898	0.297	26.30	0.038

II. COUPLING WITH CONDUCTION BAND OF TYPE Γ_2^-

Calculating valence-band structure is complicated by the strong interaction between the various hole subbands. When T_{Body} is continuously scaled down, the hole quantization energy becomes comparable with the energy gap; therefore, possible coupling with the conduction bands should also be considered. In this work, we began with an eight-band Hamiltonian¹⁵ description, including the valence-band coupling with the conduction band of type Γ_2^- , to investigate the sufficiency of a six-band Hamiltonian¹³ approach with the parameters used listed on Table I. Figure 1 shows the comparison of hole subband structure calculated with an eight- and six-band Hamiltonian for both Si and Ge quantum wells with a $\langle 100 \rangle$ surface and a T_{Body} of 30 Å. We observed that the hole subbands structure for Ge calculated with a six-band

Hamiltonian deviates noticeably from the eight-band description, particularly for the higher subbands. From an analysis of the wave-function components for Ge subbands (see Fig. 2), it is evident that there is notable coupling with conduction band of type Γ_2^- for energy subband $n=2$, contributing to about 10% of the probability function. From this, we may conclude that an eight-band Hamiltonian approach is necessary for an accurate description of Ge hole subband structure.

For our work, however, a six-band Hamiltonian approach will suffice if the biasing condition is such that the hole carriers predominantly populate only the first subband of Ge; this usually applies to electrostatics under threshold condition. Our argument is as follows:

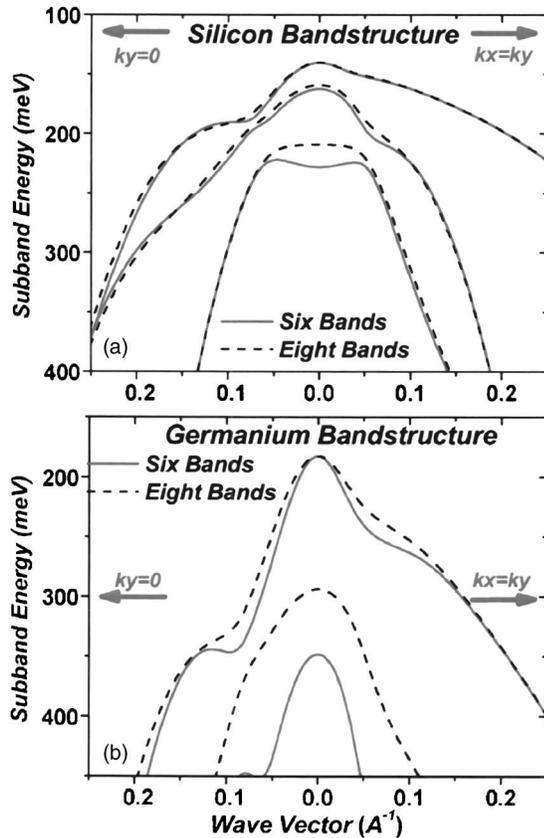


FIG. 1. Electronic hole subband structure for a 30-Å Si quantum well with $\langle 100 \rangle$ surface with an infinite energy barrier height. Calculation is done with an eight-band (see Ref. 15) and six-band (see Ref. 13) Hamiltonian for comparison. Energy plotted along wave-vector direction of $[010]$ and $[110]$. Confinement direction is taken to be along z .

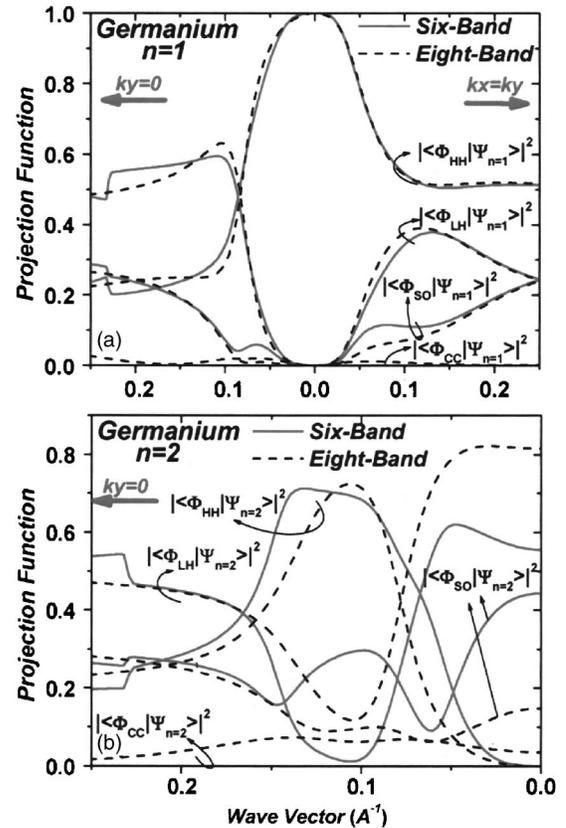


FIG. 2. Probability function projected on the various basis functions for 30-Å Ge quantum well with $\langle 100 \rangle$ surfaces, plotted for energy level (a) $n=1$ and (b) $n=2$. Calculation is done with an eight-band (see Ref. 15) and six-band (see Ref. 13) Hamiltonian for comparison. $|\psi\rangle$ is the wave function for energy subband n and $|\phi_i\rangle$ ($i=HH$: heavy hole, LH: light hole, SO: split-off hole, and CC: conduction band of type Γ_2^-) is the basis functions (Refs. 13 and 15) employed for our Hamiltonian.

- (a) At threshold condition, the Fermi energy is approximately a few kT (~ 0.025 eV; k : Boltzmann's constant and T : temperature) away from the lowest subband energy minimum, where threshold condition is usually defined to be the onset of carrier inversion. Hence, higher hole subbands can be disregarded if they are a few kT higher than the lowest subband energy minimum.
- (b) Ge generally has relatively small quantization masses, resulting in larger energy separations for the various subbands. In particular, for a 30-Å Ge quantum well with $\langle 100 \rangle$ surfaces, we have an energy separation (between $n=1$ and $n=2$) of ~ 0.1 eV.

Supported by these details, we shall adopt a six-band Hamiltonian approach in this work, exercising care when results pertaining to higher hole subbands of Ge are interpreted.

III. A NUMERICAL SOLUTION TO THE CHARGE CONTROL PROBLEM IN THE MOS SYSTEM

The numerical representation of the six-band Hamiltonian is obtained by following a discretization process outlined in Ref. 14. The six-band Hamiltonian is explicitly outlined in the Appendix where k_z is represented by its differential form $-i\partial/\partial z$ and coordinate z is taken to be the direction perpendicular to the semiconductor/oxide interface. When dealing with different crystal surface orientations of $\langle 100 \rangle$, $\langle 110 \rangle$, and $\langle 111 \rangle$, appropriate rotations of the \mathbf{k} space must be performed. Although the charge control problem in the MOS system can be solved by obtaining the self-consistent solution to the Schrödinger and Poisson equations,¹⁶ this approach is computationally intensive. In this work, we resort to the triangular-well approximation: $V(z) = eF_s z$, where F_s is the surface field and e the electronic charge. We must be aware of the limitations of the triangular-well approximation in describing MOS electrostatics under high inversion conditions,¹⁶ where the charge-screening effect will alter the potential profile significantly. Despite this, the triangular approximation is computationally efficient and expected to be qualitatively correct, thus facilitating the study of a wider range of applications.

IV. IMPACT OF ACTIVE LAYER THICKNESS AND SURFACE ORIENTATION ON HOLE QUANTIZATION EFFECT

In this section, we will examine the effect of T_{Body} on the valence-band structure of Si and Ge with a sub-5-nm T_{Body} . In Fig. 3, hole subband energies (the lowest lying at $k=0$) are plotted as a function of T_{Body} for both Si and Ge channels with various surface orientations. At a high surface field of 1 MV/cm, the sub-band energies are generally less sensitive to the decrease of T_{Body} until a certain point ($T_{\text{Body}} \sim 4$ nm for $F_s = 1$ MV/cm), where body quantization effects begin to be observed. We also noted that the energy quantization effect is strongest for $\langle 100 \rangle$ surface, followed by $\langle 111 \rangle$ and $\langle 110 \rangle$ surfaces.

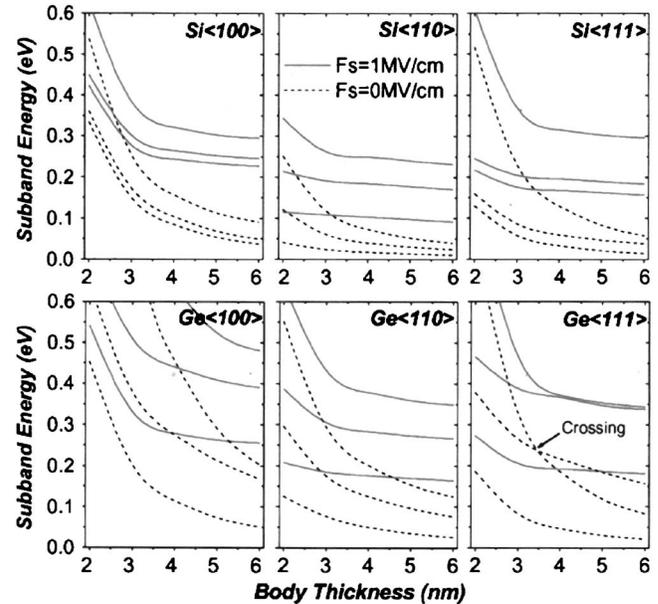


FIG. 3. Hole subband energies (at $k=0$) as function of body thickness T_{Body} , plotted for (a) Si and (b) Ge channels with various surface orientations. Surface field F_s of 1 MV/cm (bold lines) and 0 MV/cm (dashed lines) are compared. For each case, only the lowest three subbands are shown. There is apparently a crossing of the second and third subband energy for Ge $\langle 111 \rangle$ as T_{Body} is decreased.

It will be useful to provide a qualitative explanation for this observation. We begin by highlighting previous observations that the ground state of Si hole band structure are derived from the heavy-hole band.¹⁷ Figure 4 shows the equienergy surface for the heavy-hole band of bulk Si, depicting the twelve distinct prongs. A particular crystal surface with prongs more aligned to the normal of the surface will effectively yield a larger “quantization mass.” $\langle 110 \rangle$ surfaces have the prong perfectly aligned with the normal of the plane, which explains the small hole quantization effect on the $\langle 110 \rangle$ surface; this argument applies, with different results, for the $\langle 100 \rangle$ and $\langle 111 \rangle$ surfaces as well.

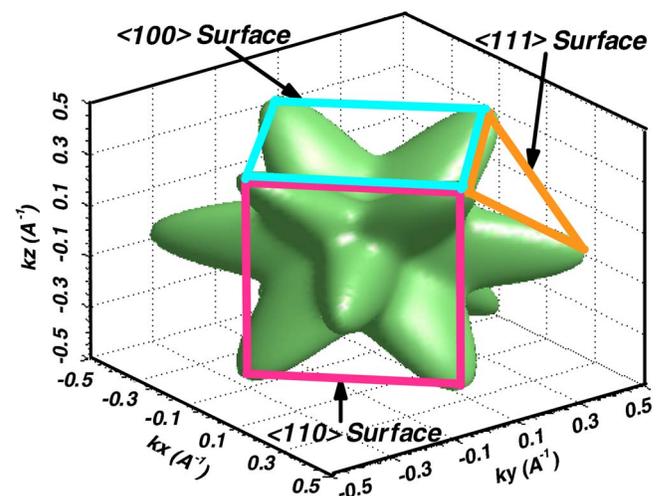


FIG. 4. Three-dimensional constant energy (at 0.1 eV reference from Γ point) surface plot for bulk Si band structure for the first valence energy band (or commonly known as heavy-hole band) depicting the twelve prominent prongs. The $\langle 100 \rangle$, $\langle 110 \rangle$, and $\langle 111 \rangle$ surface planes are illustrated and the axes are along $[100]$ direction.

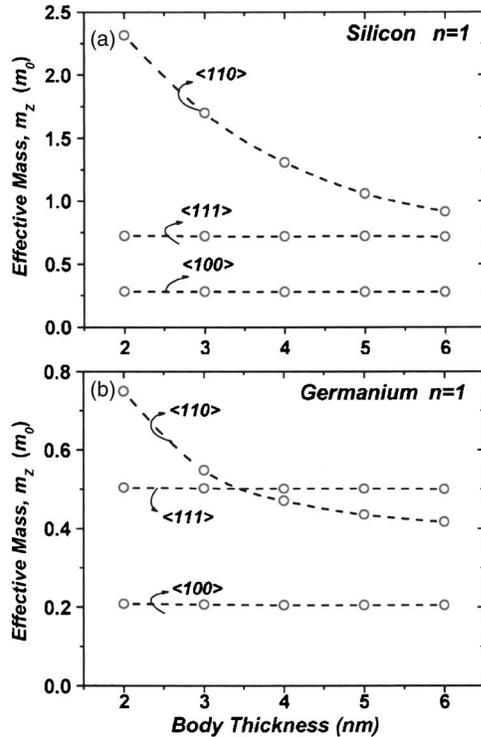


FIG. 5. Effective quantization mass m_z calculated for (a) Si and (b) Ge quantum wells by fitting the subband energies at zone-center Γ to the analytical expression for that of a quantum well; $E_0 = (\hbar^2/2m^*)(\pi/T_{\text{BODY}})^2$.

Figure 5 computes the effective quantization mass (m_z) for the ground-state subband in both the Si and Ge quantum wells under various surface orientations. This is calculated by fitting the subband energies at the zone-center Γ to the analytical expression for that of a quantum well with parabolic energy dispersion: $E_0 = (\hbar^2/2m^*)(\pi/T_{\text{BODY}})^2$. An interesting phenomenon—increasing effective quantization mass with decreasing T_{Body} for the $\langle 110 \rangle$ surface—is immediately revealed. The physical origin of this is the dependency of the valence-band mixing effect on the quantum well thickness. This effect can be analyzed by calculating the projection function, the probability function projected on the various basis functions employed for our Hamiltonian:¹³ $|\Phi_i\rangle$ ($i = \text{HH}$: heavy hole, LH: light hole, and SO: split-off hole). Figure 6(a) illustrates the projection functions of the Si $\langle 110 \rangle$ quantum wells with a T_{Body} of 30 and 60 Å. Evidently, the projection function at Γ has a noticeable dependency on T_{Body} , revealing an increasing mix of split-off holes with decreasing T_{Body} around the vicinity of Γ . Conversely, the projection function in the vicinity of Γ for the $\langle 100 \rangle$ (Fig. 2) and $\langle 111 \rangle$ [Fig. 6(b)] surfaces does not exhibit such anomalous characteristics. Thus, we may conclude that their m_z are independent of T_{Body} (Si $\langle 100 \rangle \sim 0.28m_0$, Si $\langle 111 \rangle \sim 0.72m_0$, Ge $\langle 100 \rangle \sim 0.21m_0$, and Ge $\langle 111 \rangle \sim 0.50m_0$).

V. ENERGY DISPERSION AND ANISOTROPY

Anisotropic energy dispersion and its effect on transport anisotropy in Si MOSFETs have been investigated theoretically.¹⁴ There are also experimental studies of its transport characteristics in both the low-field^{18,19} and high-field regime.²⁰ However, a study of hole energy dispersion

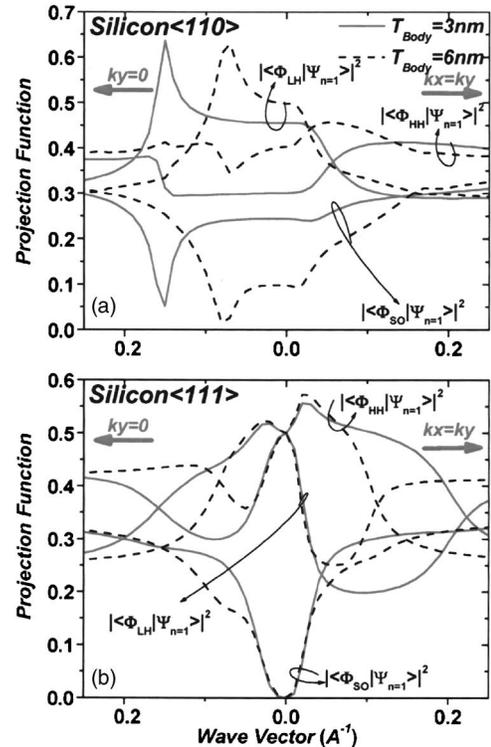


FIG. 6. Probability function projected on the various basis functions for 30 Å (bold line) and 60 Å (dashed line) Si quantum well, plotted for the first hole subband, with (a) $\langle 110 \rangle$ and (b) $\langle 111 \rangle$ surfaces. Calculation is done with a six-band (see Ref. 13) Hamiltonian. $|\psi_n\rangle$ is the wave function for energy subband n and $|\phi_i\rangle$ ($i = \text{HH}$: heavy hole, LH: light hole, and SO: split-off hole) is the basis functions (see Ref. 13) employed for our Hamiltonian.

anisotropy and its dependency on film thickness have not yet been conducted. Energy dispersion for the first two hole subbands of Si (Fig. 7) and Ge (Fig. 8) are plotted for two particular conditions as follows: (i) Bulk $F_s = 1$ MV/cm and $T_{\text{Body}} = 100$ nm, shown on the right and (ii) UTB $F_s = 1$ MV/cm and $T_{\text{Body}} = 3$ nm, shown on the left. Of particular interest are the following observations:

- (1) $\langle 100 \rangle$ surface orientation: The energy dispersion characteristics of Si $\langle 100 \rangle$ for both bulk and UTB devices [as depicted in Fig. 7(a)] look similar except with a larger uplift of the $n=2$ subband for the UTB device due to the body quantization effect. The ground-state energy ($n=1$) for Si $\langle 100 \rangle$ maintains its strong anisotropy with the decrease of T_{Body} to 3 nm, presenting an optimum channel direction (smallest m_c along $[100]$ as elucidated in Figs. 7(a) and 9(a). The $n=2$ subband presents an apparent optimum channel direction along $[110]$. The anisotropy of the two subbands may neutralize each other, rendering the observed transport characteristics relatively isotropic. This is, in fact, the experimental observation for bulk Si MOSFETs.¹⁹ However, the increased body quantization effect in UTB MOSFETs will result in carrier occupation dominance of the ground-state energy and it is very likely that the current anisotropy characteristics, due to the $n=1$ subband may ultimately manifest. For Ge $\langle 100 \rangle$, it is noted in Fig. 9(b) that its energy anisotropy is less severe than Si $\langle 100 \rangle$, with a significant

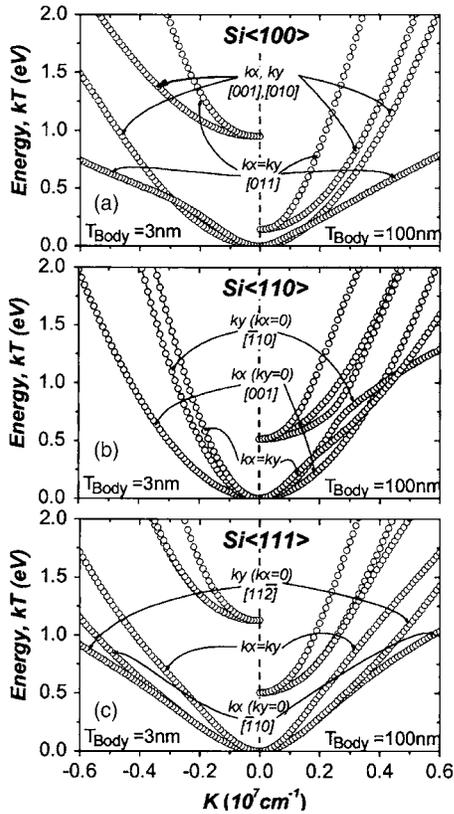


FIG. 7. Energy dispersion of Si (sub-band E_1 and subband E_2) plotted at surface field $F_S=1$ MV/cm for $T_{\text{Body}}=100$ nm (right) and $T_{\text{Body}}=3$ nm (left). For $\langle 100 \rangle$ and $\langle 110 \rangle$ surface, k_x is parallel to $[001]$ channel direction. For $\langle 111 \rangle$ surface, k_x is parallel to $[110]$ direction.

relaxation of the energy anisotropy of ground-state energy as T_{Body} is decreased.

- (2) $\langle 110 \rangle$ surface orientation: In Sec. IV, we noted the dependency of the valence-band mixing effect on the quantum well thickness for $\langle 110 \rangle$ surface thin film and its effect on m_z . It can be anticipated that this dependency of valence-band mixing effect on the quantum well thickness will also have an important effect on the energy dispersion characteristics for the $\langle 110 \rangle$ surface. Figures 7(b) and 8(b) depict a notable change in the energy dispersion of the $n=1$ subband for Si $\langle 110 \rangle$ and Ge $\langle 110 \rangle$, respectively, as the T_{Body} is decreased to 3 nm. Specifically, this change is an increase of the energy gradient drawn along the k_y (at $k_x=0$, this is the $[011]$ channel direction) and $k_x=k_y$ directions. The main effect of this will be in its carrier velocity, as elucidated in Fig. 10, which plots the radial carrier velocity $[\mathbf{v}(\mathbf{k}) = \hbar^{-1} \partial E / \partial \mathbf{k}]$ where the energy derivative is taken along the radial direction] of $n=1$ subband for both the (a) bulk and (b) UTB devices. A significantly higher intensity for carrier velocity is observed in the UTB device than in its bulk counterpart. Recently, it was experimentally observed that the optimum low-field mobility direction for Si UTB devices with a $\langle 110 \rangle$ surface is along the $[011]$ channel direction (see Fig. 11 of Ref. 14). For Si $\langle 110 \rangle$ bulk MOSFETs, it was also experimentally found that the anisotropy characteristic of low-field mobility is not significant.¹⁸ These experimental observa-

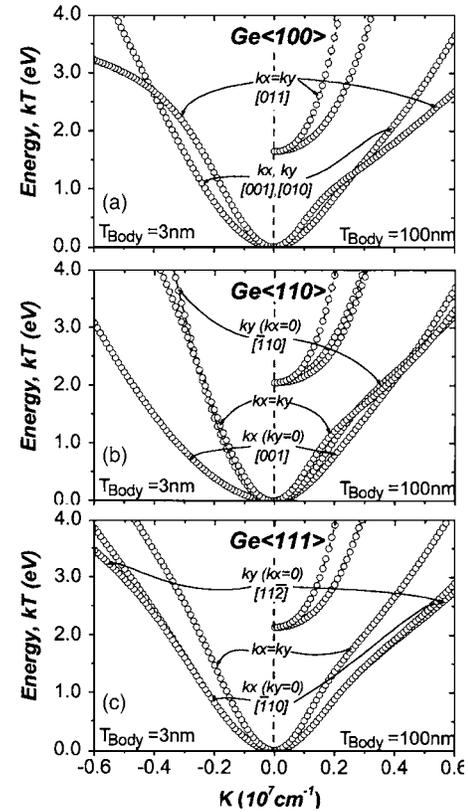


FIG. 8. Energy dispersion of Ge (subband E_1 and subband E_2) plotted at surface field $F_S=1$ MV/cm for $T_{\text{Body}}=100$ nm (right) and $T_{\text{Body}}=3$ nm (left). For $\langle 100 \rangle$ and $\langle 110 \rangle$ surface, k_x is parallel to $[001]$ channel direction. For $\langle 111 \rangle$ surface, k_x is parallel to $[110]$ direction. E_2 subband energy for $T_{\text{Body}}=3$ nm is too high to be shown in the figure.

tions correlate with our theoretical calculations and should also qualitatively apply to Ge $\langle 110 \rangle$ since its energy dispersion characteristics are similar to Si $\langle 110 \rangle$.

VI. IMPACT OF SURFACE ORIENTATION ON DENSITY OF STATES

Figure 11 plots the 2D density of states for Si and Ge thin films with a T_{Body} of 3 nm. Density of states for Ge are several times smaller than for its Si counterpart, with the $\langle 110 \rangle$ surface having the smallest density of states, followed by the $\langle 111 \rangle$ and then $\langle 100 \rangle$. From a density-of-states point of view, the employment of Ge $\langle 110 \rangle$ crystal for the device's active layer will be helpful in achieving a high-mobility channel.

VII. CONCLUSIONS

In summary, our examination of the impact of film thickness on the hole subband structure of Si and Ge thin films within the framework of kp approximation via the Luttinger–Kohn Hamiltonian has shown an anomalous increase of “effective quantization mass” for the $\langle 110 \rangle$ surface as T_{Body} is decreased. This phenomenon is due to the body-thickness-dependent valence-band mixing effect in vicinity of the zone-center Γ . The other two orientations exhibit relatively constant effective quantization mass as T_{Body} is decreased, with Ge having a consistently smaller effective quantization

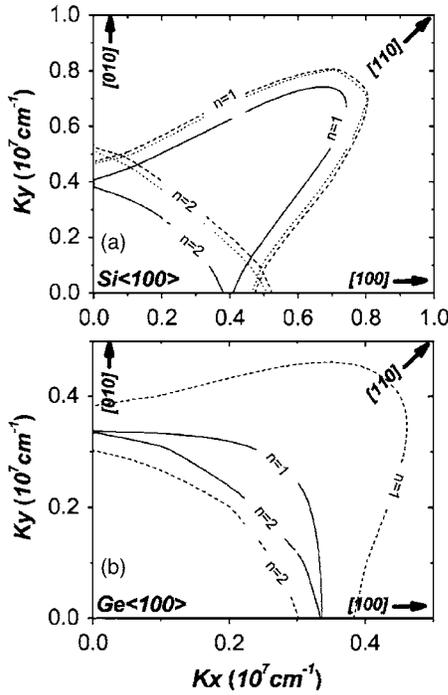


FIG. 9. Equienergy lines for the first two hole subbands of (a) Si<100> and (b) Ge<100> plotted at energy ($E-E_i$, $i=1,2$) of 25, and 50 meV, respectively, under (i) bulk high-field conditions: $F_S=1 \text{ MV/cm}$ and $T_{\text{Body}}=100 \text{ nm}$, represented by solid lines and (ii) UTB high-field conditions: $F_S=1 \text{ MV/cm}$ and $T_{\text{Body}}=3 \text{ nm}$, represented by dashed lines.

mass than its Si counterpart. It has also been observed that energy dispersion anisotropy exhibits a dependence on film thickness, especially for the <110> surface. In particular, its radial carrier velocity along the [011] channel increases as

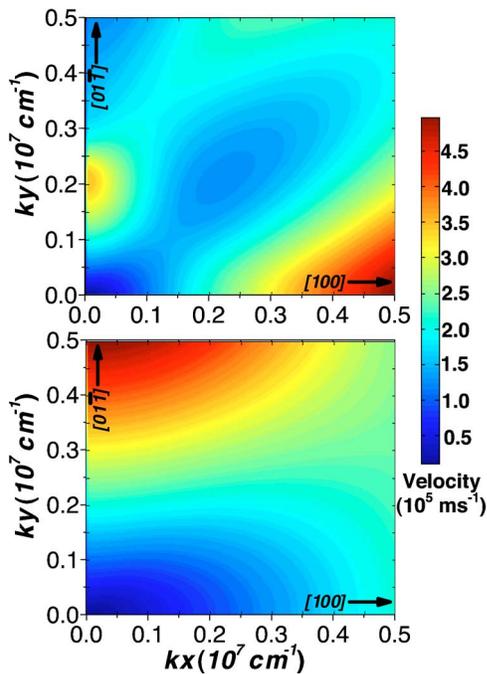


FIG. 10. Intensity plot for hole carrier radial velocity of different in-plane wave vector. Plotted for the ground-state energy of Si<110> for (a) $T_{\text{Body}}=100 \text{ nm}$ and (b) $T_{\text{Body}}=3 \text{ nm}$ at $F_S=1 \text{ MV/cm}$. Radial velocity $v(k) = \hbar^{-1} \partial E / \partial k$, is obtained by taking the gradient of its energy dispersion in the radial direction.

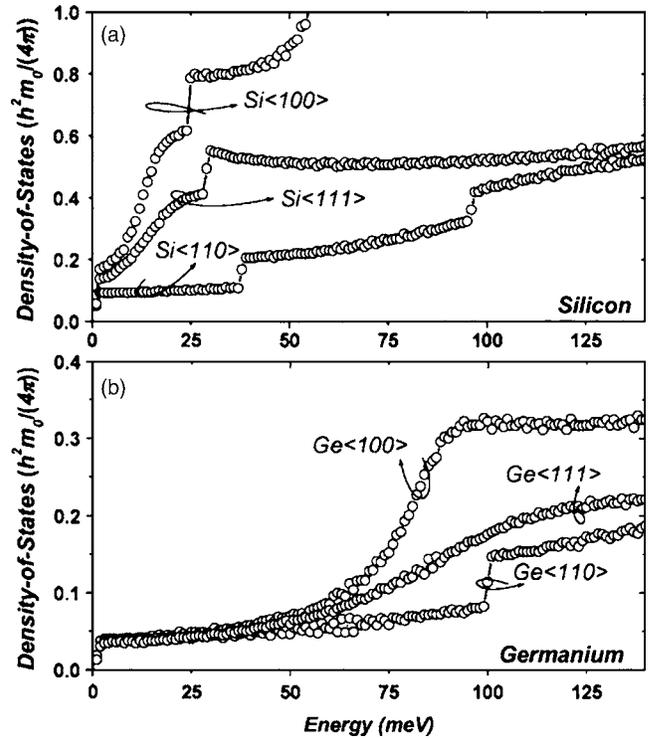


FIG. 11. Density of states for (a) Si and (b) Ge quantum wells for a particular spin state at $F_S \sim 0.1 \text{ MV/cm}$ and $T_{\text{Body}}=3 \text{ nm}$. Contributions from all the subbands are summed.

the T_{Body} is decreased. Calculated density of states of Ge thin film are several times smaller than its Si counterpart, indicating that Ge should prove advantageous for the implementation of high-mobility channels. These findings should provide useful guidelines for the design of UTB p -MOSFETs.

ACKNOWLEDGMENTS

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APPENDIX

The basis functions employed for Kohn-Luttinger Hamiltonian¹³ are depicted as follows:

$$\left| \frac{3}{2}, \frac{3}{2} \right\rangle = \frac{1}{\sqrt{2}} |x\rangle \uparrow + \frac{1}{\sqrt{2}} |y\rangle \uparrow,$$

$$\left| \frac{3}{2}, \frac{1}{2} \right\rangle = i \frac{1}{\sqrt{6}} |x\rangle \downarrow - \frac{1}{\sqrt{6}} |y\rangle \downarrow - i \frac{\sqrt{2}}{\sqrt{3}} |z\rangle \uparrow,$$

$$\left| \frac{3}{2}, -\frac{1}{2} \right\rangle = \frac{1}{\sqrt{6}} |x\rangle \uparrow - i \frac{1}{\sqrt{6}} |y\rangle \uparrow + \frac{\sqrt{2}}{\sqrt{3}} |z\rangle \downarrow,$$

$$\left| \frac{3}{2}, -\frac{3}{2} \right\rangle = i \frac{1}{\sqrt{2}} |x\rangle \downarrow + \frac{1}{\sqrt{2}} |y\rangle \downarrow,$$

$$\left| \frac{1}{2}, \frac{1}{2} \right\rangle = \frac{1}{\sqrt{3}} |x\rangle\downarrow + i \frac{1}{\sqrt{3}} |y\rangle\downarrow + \frac{1}{\sqrt{3}} |z\rangle\uparrow,$$

$$\left| \frac{1}{2}, -\frac{1}{2} \right\rangle = -i \frac{1}{\sqrt{3}} |x\rangle\uparrow - \frac{1}{\sqrt{3}} |y\rangle\uparrow + i \frac{1}{\sqrt{3}} |z\rangle\downarrow.$$

Where the functions $|X\rangle$, $|Y\rangle$, and $|Z\rangle$ are the basis functions of Γ_4 representation of the tetrahedral point group. The above choice of basis functions allows us to diagonalize the well-known spin-orbit coupling term, H_{SO} [see for, e.g., Ref. 13 eq. (V.1)]. Hence the Kohn–Luttinger Hamiltonian is

$$\begin{bmatrix} \text{HH} & \alpha & \beta & 0 & \frac{i\alpha}{\sqrt{2}} & -i\sqrt{2}\beta \\ \alpha^* & \text{LH} & 0 & \beta & \kappa & i\frac{\sqrt{3}}{\sqrt{2}}\alpha \\ \beta^* & 0 & \text{LH} & -\alpha & -i\frac{\sqrt{3}}{\sqrt{2}}\alpha^* & \kappa \\ 0 & \beta^* & -\alpha^* & \text{HH} & -i\sqrt{2}\beta^* & -\frac{i\alpha}{\sqrt{2}} \\ \frac{i\alpha^*}{\sqrt{2}} & \kappa^* & i\frac{\sqrt{3}}{\sqrt{2}}\alpha & i\sqrt{2}\beta & \text{SO} - \lambda & 0 \\ i\sqrt{2}\beta^* & -i\frac{\sqrt{3}}{\sqrt{2}}\alpha^* & \kappa^* & \frac{i\alpha}{\sqrt{2}} & 0 & \text{SO} - \lambda \end{bmatrix},$$

where:

$$\text{HH} \equiv \frac{\hbar^2}{2m} [(\gamma_1 + \gamma_2)(k_x^2 + k_y^2) + (\gamma_1 - 2\gamma_2)(k_z^2)],$$

$$\text{LH} = \frac{\hbar^2}{2m} [(\gamma_1 - \gamma_2)(k_x^2 + k_y^2) + (\gamma_1 + 2\gamma_2)k_z^2],$$

$$\text{so} = \frac{\hbar^2}{2m} [\gamma_1(k_x^2 + k_y^2 + k_z^2)],$$

$$\alpha \equiv \frac{\hbar^2}{2m} [-i2\sqrt{3}\gamma_3(k_x - ik_y)k_z],$$

$$\beta \equiv \frac{\hbar^2}{2m} [\sqrt{3}\gamma_2(k_x^2 - k_y^2) - i2\sqrt{3}\gamma_3k_xk_y],$$

$$\kappa \equiv \frac{\hbar^2}{2m} i\sqrt{2}\gamma_2[-(k_x^2 + k_y^2) + 2k_z^2],$$

where λ is the spin-orbit splitting.

For $\langle 110 \rangle$ surface, a rotation of the original \mathbf{k} space is required:

$$k'_x = k_x,$$

$$k'_y = \frac{1}{\sqrt{2}}k_y + \frac{1}{\sqrt{2}}k_z,$$

$$k'_z = -\frac{1}{\sqrt{2}}k_y + \frac{1}{\sqrt{2}}k_z,$$

and similarly for $\langle 111 \rangle$ surface:

$$k'_x = \sqrt{\frac{2}{3}}k_x - \frac{1}{\sqrt{6}}k_y + \frac{1}{\sqrt{6}}k_z,$$

$$k'_y = \frac{1}{\sqrt{2}}k_y + \frac{1}{\sqrt{2}}k_z,$$

$$k'_z = -\frac{1}{\sqrt{3}}k_x - \frac{1}{\sqrt{3}}k_y + \frac{1}{\sqrt{3}}k_z.$$

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